Lecture 8

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I. QUANTIZATION OF ELECTRICAL NETWORKS

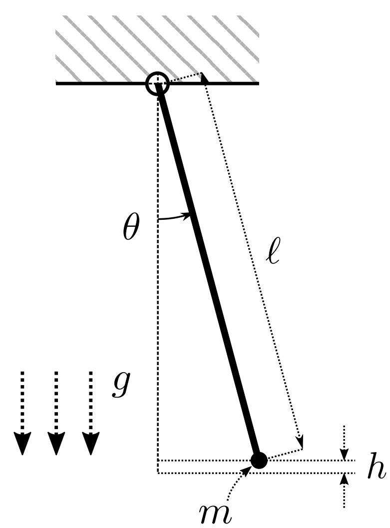
A general introduction to quantum mechanics including quantization of a harmonic oscillator is [1], for example. See [2] for quantum LC circuits in the context of superconducting qubits.

DiVincenzo's Criteria:

1. A scalable physical system with well characterized qubit
2. The ability to initialize the state of the qubits to a simple fiducial state
3. Long relevant decoherence times
4. A "universal" set of quantum gates
5. A qubit-specific measurement capability

A. Harmonic Oscillator

The harmonic oscillator is an important primer for studying quantum circuits. In particular, we will see that the canonical position and momentum in a classical harmonic oscillator are analogues of charge and flux in an LC circuit.



We consider a pendulum of length ℓ and mass m that subtends an angle θ with respect to the center. The kinetic energy is $T = \frac{1}{2}mv^2 = \frac{1}{2}m\ell^2\dot{\theta}^2$, and the potential energy is $V = mgh$, where $h = (1-\cos\theta)\ell$. Considering only small θ, we have $h \approx (1-1+\frac{\theta^2}{2})\ell = \ell\frac{\theta^2}{2}$. Therefore, the potential energy is $V = \frac{1}{2}mg\ell\theta^2$. The Lagrangian $L \equiv T - V$ of our system is

$$L = \frac{1}{2}m\ell^2\dot{\theta}^2 - \frac{1}{2}mg\ell\theta^2 \tag{1}$$

Let us take θ as the generalized coordinate. Then the corresponding generalized momentum is

$$p \equiv \frac{\partial L}{\partial \dot{\theta}} \approx \frac{\partial}{\partial \dot{\theta}}\Big(\frac{1}{2}m\ell^2\dot{\theta}^2 - \frac{mg\ell}{2}\theta^2\Big) = m\ell^2\dot{\theta}. \tag{2}$$

Note that p is nothing but the angular momentum.

The Euler-Lagrange equation is

$$\frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{\theta}}\Big) - \frac{\partial L}{\partial \theta} = 0. \tag{3}$$

By substituting $p = \partial L/\partial \dot{q}$ and noting that $\partial L/\partial\theta = -\partial V/\partial\theta$, we have Newton's equation of motion

$$\frac{dp}{dt} = -\frac{\partial V}{\partial \theta}\ . \tag{4}$$

Now, inserting $p = m\ell^2\dot{\theta}$, we have

$$m\ell^2\ddot{\theta} + mg\ell\theta = 0\ , \tag{5}$$

i.e., the equation of motion:

$$\ddot{\theta} + \frac{g}{\ell}\theta = 0. \tag{6}$$

Taking as a usual trial function $\theta = C\exp(i\omega t)$, where $C \neq 0$ is a constant, and ω is the angular frequency, Eq. (6) becomes:

$$\Big(-\omega^2 + \frac{g}{\ell}\Big)C\exp(i\omega t) = 0\ . \tag{7}$$

This is valid at all t if and only if

$$-\omega^2 + \frac{g}{\ell} = 0. \tag{8}$$

This is the so-called characteristic polynomial of the linearized equation of motion. Solving for ω we find the natural angular frequency of small oscillation of the pendulum:

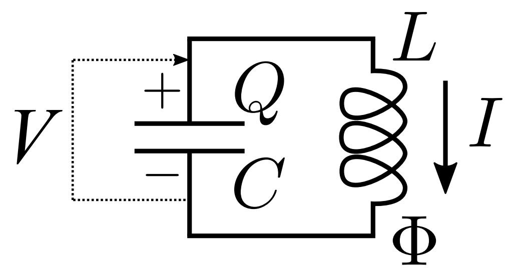
$$\omega = \sqrt{g/\ell}\ . \tag{9}$$

We have derived the eigenfrequency of the system by solving the Euler-Lagrange equation (6).

B. Superconducting LC oscillator

Once you understand the harmonic oscillator, you can easily apply the concept to a superconducting LC circuit.

Let us consider a classical superconducting LC circuit. The electrical energy will oscillate between the kinetic energy stored in the capacitor C, and the potential energy associated with the magnetic flux in the coil $\Phi = LI$, where L is the inductance of the coil, and $I = \dot{Q}$ is the current.



From the above circuit, we also see that the voltage drop across the inductor is V; hence, from Lenz's law we have $\dot{\Phi} = V$. Therefore,

$$V = L\dot{I} \tag{10}$$

Since the instantaneous power fed into an electric circuit is simply the product of the voltage across circuit V times the current I flowing into the positive voltage node, we have

$$P = V\dot{Q}. \tag{11}$$

The electrical energy stored in the capacitor is

$$T = \int_{t_0}^{t_1} P dt = \int_{t_0}^{t_1} V I dt = \int_{t_0}^{t_1} V C \dot{V} dt = \int_0^V V' C dV' = \frac{1}{2} C V^2 = \frac{C}{2}\dot{\Phi}^2. \tag{12}$$

while the electrical energy stored in the inductor is

$$U = \int_{t_0}^{t_1} P dt = \int_{t_0}^{t_1} V I dt = \int_{t_0}^{t_1} (L\dot{I}) I dt = \int_0^I L I' dI' = \frac{1}{2} L I^2 = \frac{\Phi^2}{2L}. \tag{13}$$

We take Φ as the generalized coordinate and $\dot{\Phi}$ as the corresponding generalized velocity. From Eqs. (12) and (13), we understand $T = \frac{C}{2}\dot{\Phi}^2$ is interpreted as the kinetic energy while $U = \frac{1}{2L}\Phi^2$ the potential energy. The Lagrangian is therefore

$$L = T - V = \frac{C}{2}\dot{\Phi}^2 - \frac{\Phi^2}{2L} \ . \tag{14}$$

The canonical momentum is

$$p \equiv \frac{\partial L}{\partial \dot{\Phi}} = C\dot{\Phi} = Q. \tag{15}$$

The Euler-Lagrange equation derived from the Lagrangian L is

$$C\ddot{\Phi} + \frac{\Phi}{L} = 0 \rightarrow \ddot{\Phi} + \frac{1}{LC}\Phi = 0, \tag{16}$$

which shows the natural angular frequency of oscillations is

$$\omega = \frac{1}{\sqrt{LC}}. \tag{17}$$

Compare this with $\omega = \sqrt{g/\ell}$ for the pendulum.

To summarize, the pendulum and LC oscillator correspondences are

$$\begin{array}{rcl} \text{Position} \quad x & \longleftrightarrow & \text{Flux} \quad \Phi \\ \text{Momentum} \quad p & \longleftrightarrow & \text{Charge} \quad Q \\ \text{Mass} \quad m & \longleftrightarrow & \text{Capacitance} \quad C \\ \text{Resonance frequency} \quad \omega = \sqrt{\frac{g}{\ell}} & \longleftrightarrow & \omega = \sqrt{\frac{1}{LC}} \end{array}$$

C. Legendre transformation to Hamiltonian

We must find the Hamiltonian describing the LC circuit to write down the Schrödinger equation of the system. The Lagrangian L is a function of the coordinate Φ and the velocity $\dot{\Phi}$ while the Hamiltonian H is a function of the coordinate Φ and the momentum Q. This change of variables is realized by the Legendre transformation that we see below.

For a general set of canonical variables $\{p, q\}$, the Hamiltonian and the Lagrangian is related as

$$H(p, q) \equiv \dot{q}p - L(\dot{q}, q). \tag{18}$$

We take the total time derivative of H to analyze the system dynamically as

$$\frac{dH}{dt} = \ddot{q}p + \dot{q}\dot{p} - \frac{\partial L}{\partial q}\dot{q} - \frac{\partial L}{\partial \dot{q}}\ddot{q} - \frac{\partial L}{\partial t}. \tag{19}$$

Further, we note that $p \equiv \partial L/\partial \dot{q}$ and L has no explicit time-dependence. Then the total time derivative of the Hamiltonian becomes

$$\frac{dH}{dt} = \ddot{q}p + \dot{q}\dot{p} - \frac{\partial L}{\partial q}\dot{q} - p\ddot{q} = \dot{q}\left[\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q}\right] = 0. \tag{20}$$

That is to say, the Hamiltonian is a constant of motion.

In terms of our generalized coordinate Φ and generalized momentum Q, Eq. (18) is

$$H = Q\dot{\Phi} - \left(\frac{C}{2}\dot{\Phi}^2 - \frac{\Phi^2}{2L}\right) = \frac{Q^2}{2C} + \frac{\Phi^2}{2L}. \tag{21}$$

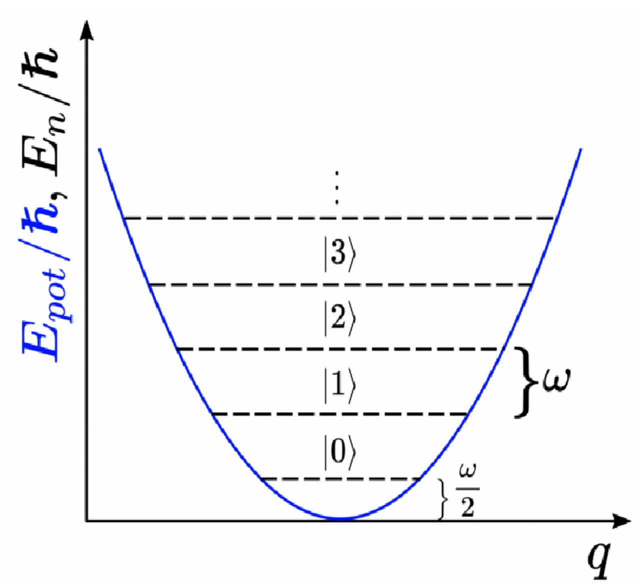
Note that the first term is the energy of a capacitor while the second term that of an inductor. The Hamiltonian therefore represents the total energy of the system.

$$H = T + V. \tag{22}$$

The energy of the system is conserved in view of Eq. (20).

We have derived the total energy of the system starting from the Lagrangian. This is necessary to analyze the LC circuit quantum mechanically as we see in the following.

D. Quantization of Harmonic Oscillator



We see below that the energy of a quantum harmonic oscillator takes discrete values $\hbar\omega(n + 1/2)$, on the contrary to a classical harmonic oscillator. For an LC circuit, it implies the excitation is made of a collection of quanta with the energy unit $\hbar\omega$. In other words, electromagnetic field of the LC circuit is quantized and hence the energy E is quantized.

- In a harmonic oscillator, the energy is quantized <u>equidistantly</u>.

- Energy quantization can be seen as counting the number of photons stored in the oscillator.

In quantum mechanics, variables are replaced by operators, i.e.

$$q \to \hat{q}, \quad p \to \hat{p}.$$

We will use $\hat{}$ to denote an operator, some examples being the charge $\hat{Q}$ and the flux $\hat{\Phi}$.

For practical reasons, we often use matrix representations, e.g.,

$$Q_{k\ell} = \langle e_k|\hat{Q}|e_\ell\rangle,$$

where $\{|e_k\rangle\}$ is the set of basis vectors of the Hilbert space. Generically, an operator acting on a state is regarded as a matrix acting on a vector and may be represented as

$$\begin{pmatrix} (O\psi)_1 \\ (O\psi)_2 \\ \vdots \\ (O\psi)_i \\ \vdots \end{pmatrix} = \begin{pmatrix} O_{11} & O_{12} & \cdots & O_{1j} & \cdots \\ O_{21} & O_{22} & \cdots & O_{2j} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ O_{i1} & O_{i2} & \cdots & O_{ij} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_j \\ \vdots \end{pmatrix} \tag{23}$$

Two canonically conjugate variables obey the commutation relation

$$[\hat{p}, \hat{q}] \equiv \hat{p}\hat{q} - \hat{q}\hat{p} = -i\hbar. \tag{24}$$

Let us find the spectrum of a harmonic oscillator whose Hamiltonian is

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2. \tag{25}$$

We diagonalize $\hat{q}$ and treated as a classical variable q while $\hat{p} = (\hbar/i)d/dq$. It turns out to be convenient to introduce operators $\hat{a}$ and $\hat{a}^\dagger$ defined as

$$\hat{q} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger), \quad \hat{p} = -i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a} - \hat{a}^\dagger), \tag{26}$$

namely,

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{q} + i\sqrt{\frac{1}{2m\hbar\omega}}\hat{p}, \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{q} - i\sqrt{\frac{1}{2m\hbar\omega}}\hat{p}. \tag{27}$$

By noting the commutation relation (exercise)

$$[\hat{a}, \hat{a}^\dagger] = 1, \tag{28}$$

it is easy to show

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 = \frac{1}{2}\hbar\omega(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger) = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right). \tag{29}$$

The spectrum of the harmonic oscillator is easily found. Let $\hat{n} = a^\dagger a$ and $|n\rangle$ be an eigenvector of $\hat{n}$ such that $\hat{n}|n\rangle = n|n\rangle$. From the commutation relations $[\hat{n}, \hat{a}] = -\hat{a}$ and $[\hat{n}, \hat{a}^\dagger] = \hat{a}^\dagger$, it is easy to show

$$\hat{n}(\hat{a}|n\rangle) = (n-1)\hat{(}a|n\rangle), \quad \hat{n}(\hat{a}^\dagger|n\rangle) = (n+1)(\hat{a}^\dagger|n\rangle),$$

showing $\hat{a}|n\rangle \propto |n-1\rangle$ and $\hat{a}^\dagger|n\rangle \propto |n+1\rangle$. The operator $\hat{a}$ reduces the eigenvalue n by 1 while $\hat{a}^\dagger$ increases the eigenvalue by 1 and they are called the annihilation and creation operators, respectively. Note that H and $\hat{n}$ are related as

$$H = \hbar\omega\left(\hat{n} + \frac{1}{2}\right). \tag{30}$$

The action of $\hat{a}^k$ on $|n\rangle$ reduces the eigenvalue n to $n-k$ but k cannot be arbitrarily large. The eigenvalue of $\hat{n}$ must be nonnegative since

$$\|\hat{a}|n-k\rangle\|^2 = \langle n-k|\hat{a}^\dagger\hat{a}|n-k\rangle = (n-k)\langle n-k|n-k\rangle = n-k \geq 0.$$

This means that $k \leq n$. This problem can be circumvented if there is a state $|0\rangle$ such that $\hat{n}|0\rangle = 0$. This implies $\langle 0|\hat{a}^\dagger\hat{a}|0\rangle = \|\hat{a}|0\rangle\|^2 = 0$, namely $\hat{a}|0\rangle = 0$, showing the state $|-1\rangle$ does not exist. Let us call this state $|0\rangle$ the "vacuum" state. All other states are created by repeated applications of $\hat{a}^\dagger$ on $|0\rangle$ as

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle \qquad (n = 0, 1, 2, \ldots) \tag{31}$$

where $\sqrt{n!}$ takes care of the normalization (exercise, use $\langle n|\hat{a}\hat{a}^\dagger|n\rangle = n+1$).

Let us evaluate the matrix elements of $\hat{a}$ and $\hat{a}^\dagger$ next. We find

$$\langle m|\hat{a}|n\rangle = \sqrt{n}\langle m|n-1\rangle = \sqrt{n}\delta_{m,n-1} \tag{32}$$

and

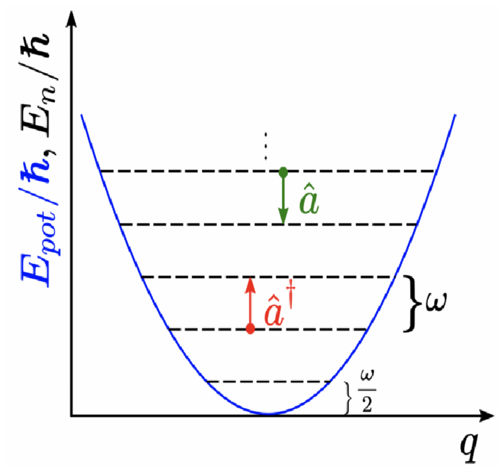
$$\langle m|\hat{a}^\dagger|n\rangle = \sqrt{n+1}\langle m|n+1\rangle = \sqrt{n+1}\delta_{m,n+1}. \tag{33}$$

Explicitly they have matrix expressions

$$\hat{a}^\dagger = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & \cdots \\ \sqrt{1} & 0 & 0 & \cdots & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \cdots & 0 & \cdots \\ 0 & 0 & \sqrt{3} & \cdots & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \cdots \\ \vdots & \vdots & \vdots & \cdots & \sqrt{n} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{34}$$

$$\hat{a} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots & 0 & \cdots \\ 0 & 0 & 0 & 0 & \ddots & \vdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \cdots & \sqrt{n} & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & \ddots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{35}$$

$$\hat{n} = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots & 0 & \cdots \\ 0 & 0 & 2 & 0 & \cdots & 0 & \cdots \\ 0 & 0 & 0 & 3 & \ddots & \vdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \cdots & n & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & \ddots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{36}$$



In summary, the eigenvalues of a harmonic oscillator are quantized as

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \qquad n = 0, 1, 2 \ldots. \tag{37}$$

The difference between the adjacent eigenvalues is a constant $\hbar\omega$ independent of n. The operator $\hat{a}$ shifts the eigenvalue downward by $\hbar\omega$, while $\hat{a}^\dagger$ shifts the eigenvalue upward by $\hbar\omega$. There is the lowest energy vacuum state $|0\rangle$. The eigenvalue $E_0 = \hbar\omega/2$ is called the vacuum energy or the zero-point energy. E_0 cannot vanish because of the uncertainty principle. There is no state such that $\hat{p}|\psi\rangle = \hat{q}|\psi\rangle = 0$ simultaneously.

Let us estimate the zero-point energy from uncertainty relation point of view. Let $\Delta A \equiv \sqrt{\langle\psi|A^2|\psi\rangle - \langle\psi|A|\psi\rangle^2}$ be the standard deviation of an observable A with respect to some state $|\psi\rangle$. The uncertainty relation tells us that

$$\Delta p \Delta q \geq \frac{1}{2}|\langle\psi|[p, q]|\psi\rangle| = \frac{\hbar}{2}.$$

Let us assume the inequality is saturated for the ground state $|0\rangle$; $\Delta p \Delta q = \hbar/2$, or

$$(\Delta p)^2(\Delta q)^2 = \frac{\hbar^2}{4}. \tag{38}$$

By substituting $(\Delta p)^2 = \hbar^2/4(\Delta q)^2$ into the Hamiltonian, we obtain

$$H = \frac{\hbar^2}{8m(\Delta q)^2} + \frac{1}{2}m\omega^2(\Delta q)^2. \tag{39}$$

H is minimized when

$$\frac{\partial H}{\partial(\Delta q)^2} = -\frac{\hbar^2}{8m(\Delta q)^4} + \frac{1}{2}m\omega^2 = 0,$$

from which we obtain

$$(\Delta q)^2 = \frac{\hbar}{2m\omega}. \tag{40}$$

By substituting this into our Hamiltonian, we obtain

$$H = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{1}{2}\hbar\omega \tag{41}$$

as promised.

E. Quantization of the LC oscillator

For the superconducting resonator, we have

$$\hat{H} = \frac{\hat{Q}^2}{2C} + \frac{\hat{\Phi}^2}{2L} = \frac{\hat{Q}^2}{2C} + \frac{1}{2}C\omega^2\hat{\Phi}^2, \tag{42}$$

where $\omega = 1/\sqrt{LC}$. Following the above prescription, we introduce $\hat{a}$ and $\hat{a}^\dagger$ as

$$\hat{\Phi} = \sqrt{\frac{\hbar}{2C\omega}}\left(\hat{a} + \hat{a}^\dagger\right), \quad \hat{Q} = -i\sqrt{\frac{\hbar C\omega}{2}}\left(\hat{a} - \hat{a}^\dagger\right). \tag{43}$$

Equation (42) is put in the standard form as

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right). \tag{44}$$

This tells us that the total energy of the system is the sum of the number of photons stored at frequency ω and the vacuum fluctuations $(+1/2)$.

F. Problem of LC circuit

You might think you could use the LC circuit as a qubit by taking the Hilbert space spanned by $|0\rangle$ and $|1\rangle$. However this is not the case. Transition between $|0\rangle$ and $|1\rangle$ is realized by absorption/emission of a photon of energy $\hbar\omega$. Since the energy eigenvalues of a harmonic oscillator are equidistant, the same photon induces transition between arbitrary $|n\rangle$ and $|n \pm 1\rangle$ and it is impossible to confine the qubit state within $\text{Span}\{|0\rangle, |1\rangle\}$.

This problem is circumvented by introducing nonlinearity in the potential energy $V(\Phi)$. We see in the following lectures that this will be realized by replacing the inductor in the LC circuit with a Josephson junction.

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[1] J. J. Sakurai and J. Napolitano, Modern Quantum Mechanics (2nd ed), Cambridge University Press, 2017.

[2] D. D. Stancil and G. T. Byrd, Principles of Superconducting Quantum Computers, Wiley, 2022.